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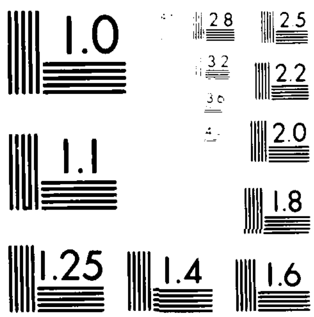

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Two of the most commonly used methods, the Trapezoidal Rule and the two-step backward differentiation formula, both have drawbacks when applied to difficult stiff problems. The Trapezoidal Rule does not sufficiently damp the stiff components and the backward differentiation method is unstable for rapidly varying steps. In this paper we show that there exists a one-parameter family of two-steps, second-order one-leg methods which are stable for any test problem, using arbitrary step sequences.

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STABILITY OF TWO-STEP METHODS FOR VARIABLE INTEGRATION STEPS

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ABSTRACT: Two of the most commonly used methods, the Trapezoidal Rule and the two-step backward differentiation formula, both have drawbacks when applied to difficult stiff problems. The Trapezoidal Rule does not sufficiently damp the stiff components and the backward differentiation method is unstable for rapidly varying steps. In this paper we show that there exists a one-parameter family of two-steps, second-order one-leg methods which are stable for any test problem $\dot{x} = \lambda(t)x$, $Re\ \lambda(t) \leq 0$, using arbitrary step sequences.

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1. Introduction

This paper is concerned with the numerical integration of differential systems,

$$\dot{x} = f(t, x), \tag{1.1}$$

by linear multistep and one-leg methods. On a uniform grid $t_n = nh$, $n = 0, 1, \ldots, h > 0$, a linear multistep (MS) method of step number k,

$$\sum_{j=0}^{k} \alpha_j x_{n+j} - h \sum_{j=0}^{k} \beta_j f(t_{n+j}, x_{n+j}) = 0, \tag{1.2}$$

is defined by a set of constant coefficients $\{\alpha_j, \beta_j\}$, $j = 0, \ldots, k$. Throughout this paper it will be assumed that (1.2) is normalized by the constraint

$$\sum_{j=0}^{k} \beta_j = 1. \tag{1.3}$$

Using the familiar polynomials $\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j$ and $\sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j$, and the shift operator E defined by $x_{n+1} = Ex_n$, the method (1.2) can be written in the form

$$\rho(E)x_n - h\sigma(E)f(t_n, x_n) = 0, \tag{1.4}$$

with the normalization

$$\sigma(E)1 = 1. \tag{1.5}$$

On a variable grid $\{t_0, t_n = t_0 + \sum_{\nu=1}^{n} h_\nu, n = 1, 2, \ldots\}$, all or some of the coefficients α_j, β_j normally depend on n. For practical purposes, the MS-method in the variable step case is often written as

$$\sum_{j=0}^{k} \alpha_{j,n} x_{n+j} - h_{n+k} \sum_{j=0}^{k} \beta_{j,n} f(t_{n+j}, x_{n+j}) = 0 \tag{1.6}$$

with the normalization

$$\sum_{j=0}^{k} \beta_{j,n} = 1. \tag{1.7}$$

Equivalently it can be expressed in the form

$$\rho_n x_n - h_{n+k} \sigma_n f(t_n, x_n) = 0 \tag{1.8}$$

and the normalization as

$$\sigma_n 1 = 0, \tag{1.9}$$

where the operators ρ_n and σ_n are defined by

$$\rho_n x_n = \sum_{j=0}^{k} \alpha_{j,n} x_{n+j}, \quad \sigma_n x_n = \sum_{j=0}^{k} \beta_{j,n} x_{n+j}. \tag{1.10}$$

For theoretical derivations it is preferable to write the MS-method in terms of a step other than the forward-most step, $h_{n+k} = t_{n+k} - t_{n+k-1}$, as is done in parts of this paper.

With every MS-method one can associate its one-leg (OL) "twin" or counterpart which, for variable steps, is defined by

$$\rho_n x_n - h_{n+k} f(\sigma_n t_n, \sigma_n x_n) = 0 \tag{1.11}$$

and results from the MS-method (1.8) by permuting f with the operator σ_n. OL-methods were first introduced in [5] for theoretical purposes but were found to be useful as integration methods in their own right [19].

Our aim in this paper is to look for methods with very strong stability properties. More specifically, we seek

> methods which produce bounded solutions whenever applied to the test equation
>
> $$\dot{x} = \lambda(t)x, \quad Re\, \lambda(t) \leq 0 \tag{1.12}$$
>
> using any step sequence $\{h_n\}$.

Asking for stability with arbitrary step sequençes may seem to be too strong a requirement. However, we show that there do exist methods having this property and thus the above requirement is reasonable. For other methods stability results can be proved but only under rather complicated assumptions on the interplay between the time dependence of the problem and the step changes, [13, 20].

It was demonstrated in [19] that, if formulas are implemented in the multistep form, then unfavorable combinations of variable steps and variable coefficients in the equations can lead to instability. As a simple example of this, consider the Trapezoidal Rule:

$$x_{n+1} - x_n = \frac{1}{2} h_{n+1} (f(t_n, x_n) + f(t_{n+1}, x_{n+1})).$$

which when applied to (1.12) gives

$$x_{n+1} = [1 + \frac{1}{2}h_{n+1}\lambda(t_n)][1 - \frac{1}{2}h_{n+1}\lambda(t_{n+1})]^{-1}x_n.$$

Let $h_{2m} = \frac{1}{2}$ and $h_{2m+1} = 4$ and choose $\lambda(t)$ such that $\lambda(t_{2m}) = -1$ and $\lambda(t_{2m+1}) = 0$. Then, $x_{2m} = (-2)^m x_0$, i.e. the Trapezoidal Rule is unstable. The Implicit Midpoint Rule (one-leg "twin" of the Trapezoidal Rule),

$$x_{n+1} - x_n = h_{n+1} f(\frac{1}{2}(t_n + t_{n+1}), \frac{1}{2}(x_n + x_{n+1})),$$

on the other hand gives

$$x_{n+1} = [1 + \frac{1}{2}h_{n+1}\lambda(\frac{1}{2}(t_n + t_{n+1}))][1 - \frac{1}{2}h_{n+1}\lambda(\frac{1}{2}(t_n + t_{n+1}))]^{-1}x_n$$

so that for all problems (1.12) we have $|x_{n+1}| \le |x_n|$.

Recall that, for *constant* steps, linear multistep methods and one-leg methods have similar stability properties [6] but, as stated before, with *variable* steps this is no longer the case. Thus, although we sometimes write formulas in multistep form it should be understood that they are to be implemented in one-leg form.

For constant steps and constant λ's, our stability requirement reduces to A-stability. Therefore, the order of the methods we are looking for cannot exceed two and it is natural to restrict our attention to two-step methods. Observe that, for every given step ratio r, there exists a two-parameter family of two-step second-order formulas. To start with, consider formulas of this class whose coefficients depend smoothly on r. Choosing geometric step sequences and related time-dependent problems we show, by expanding around $r = 1$, that

> there exists at most a one-parameter family of constant-step formulas which can smoothly be extended to variable steps in such a way as to satisfy our stability requirement.

This result is demonstrated in Section 5 and was first given in [20]. The one-parameter family of constant-step formulas in question happens to be exactly to set of those second-order two-step methods which are A-contractive in the max-norm, which in turn is the same as the set of methods which are A-contractive in a monotone inner product norm (i.e., G-stable with diagonal G).

Let us recall this terminology. With *any solution* $\{x_n\}$ of the difference equation we associate the sequence $\{X_n\}$ where $X_n = (x_{n+k-1}, x_{n+k-2}, \ldots, x_n)$. We say that a method is *stable* at $q = h\lambda$ if it produces bounded solutions when applied to the test equation

$$\dot{x} = \lambda x, \quad \lambda \in C; \tag{1.13}$$

it is said to be *contractive* at $q = h\lambda$ with respect to a given norm $\|\cdot\|$ if $\|X_{n+1}\| \le \|X_n\|$, [18]. The set of stable q's is called the stability region S of the method and, similarly, the contractivity region $C_{\|\cdot\|}$ is the set of q's at which the method is contractive. The method is called A-stable (A-contractive w.r.t. a given norm) if the left half-plane is contained in $S(C_{\|\cdot\|})$, and A_0-stability (A_0-contractive) if the negative real axis is contained in $S(C_{\|\cdot\|})$. For every A-stable method there exists an inner product norm in which the method is A-contractive, [8]. Note that when a one-leg method is applied to (1.12), then $\|X_{n+1}\| \le \|X_n\|$ follows for all n and for any $\lambda(t)$ as long as $\{h\lambda(t_n)\} \subset C_{\|\cdot\|}$.

Contractivity in the max-norm was first investigated in [14] for Adams- and Runge-Kutta methods. In [1, 2] contractivity in certain polygonal norms was studied to produce variable-step stability results for backward differentiation methods. Contractivity for dissipative nonlinear systems in inner product norms (G-stability) was introduced in [5,6] and further analyzed in [7]-[11], [15]-[19]. Contractivity results for Runge-Kutta methods are given in [3,4,12].

As mentioned above, the stability analysis using geometric step sequences led to *constant*-step methods which are A-contractive in the max-norm and in a monotone inner product norm. It is therefore natural to also look for *variable*-step formulas which are A-contractive in these norms. It turns out that

for any step ratio r, there exists a one-parameter family of A-contractive methods.

Hence we have now a) characterized the set of constant-step formulas for which variable step stability results might exist, and b) given extensions of all of these formulas to variable steps which actually do preserve stability. We get the same methods using either the max-norm or diagonal G-matrices. However, the G-matrix depends on the formula parameter and for every parameter value (*i.e.* any fixed-step formula in the family) we find a unique variable-step extension which is A-contractive in the same G-norm as the constant-step formula in question. Observe that, with this extension, all results concerning error bounds for nonlinear systems carry over immediately. The max-norm, on the other hand, does not depend on the method, and therefore stability is preserved even if we pick an arbitrary A-contractive variable-step method at every step. The max-norm results were first given in [20] and are presented in Section 3, while the results using the G-stability approach were given in [10], and are presented in Section 2.

In Section 4 we analyze A_0-contractivity for variable steps and give variable-step extensions for all constant-step formulas which are A_0-contractive in the max-norm. We also briefly discuss the selection of particular methods from among the one-parameter family of A-contractive methods. Finally, we rewrite all methods in a practical parametrization and list their error constants.

2. A-contractivity in the G-norm

Consider the general variable-step k-step formula

$$\sum_{j=0}^{k} \alpha_j x_{n+j} = \bar{h}_n \sum_{j=0}^{k} \beta_j \dot{x}_{n+j} \tag{2.1}$$

with the normalization

$$\sum_{j=0}^{k} \beta_j = 1 \tag{2.2}$$

For $k \geq 2$, the coefficients α_j, β_j depend on the step ratios

$$r_{n+j} = h_{n+j}/h_{n+j-1}, \quad j = 2, \ldots, k, \tag{2.3}$$

where $h_n = t_n - t_{n-1}$, although for simplicity in writing they are not subscripted here, and $\bar{h}_n$ is some homogeneous function of the first degree of the h_{n+j}, $j = 1, \ldots, k$. The formula (2.1) can be written using the difference operators

$$\rho x_n := \sum_{j=0}^{k} \alpha_j x_{n+j}, \quad \sigma x_n := \sum_{j=0}^{k} \beta_j x_{n+j}, \tag{2.4}$$

where $\rho = \rho_n$, $\sigma = \sigma_n$. In terms of these operators, (2.1) becomes

$$\rho x_n = \bar{h}_n \sigma \dot{x}_n. \tag{2.5}$$

Two possible implementations of (2.5), as applied to

$$\dot{x} = f(t, x), \tag{2.6}$$

are the familiar linear multistep method

$$\rho x_n = \bar{h}_n \sigma f(t_n, x_n) \tag{2.7}$$

on the one hand and the one-leg method [5,6]

$$\rho x_n = \bar{h}_n f(\sigma t_n, \sigma x_n) \tag{2.8}$$

on the other hand. Necessary and sufficient conditions for the one-leg method to be of order of accuracy p were given in [10] in terms of the moments

$$M_\nu(\rho) := \sum_{j=0}^{k} \alpha_j \tau_j^\nu, \quad M_\nu(\sigma) := \sum_{j=0}^{k} \beta_j \tau_j^\nu, \quad \nu = 0, 1, \ldots, \tag{2.9}$$

where $t_{n+j} = t_n^* + \tau_j \bar{h}_n$, $j = 0, \ldots, k$, and t_n^* is some reference point. The method (2.8) is of order p iff, in addition to the familiar linear constraints

$$M_\nu(\rho) = \nu M_{\nu-1}(\sigma), \quad \nu = 0, 1, \ldots p \tag{2.10}$$

for p^{th} order accuracy of the multistep method (2.7), the nonlinear conditions

$$M_{\nu-1}(\sigma) = [M_1(\sigma)]^{\nu-1}, \quad \nu = 1, \ldots, p \tag{2.11}$$

are satisfied. For $p = 1$, (2.10) for $\nu = 0$ and 1 represents the consistency conditions

$$\begin{aligned} \rho(1) &= \sum_{j=0}^{k} \alpha_j = 0, \\ \sum_{j=0}^{k} \alpha_j \tau_j &= \sigma(1) = \sum_{j=0}^{k} \beta_j = 1, \end{aligned} \tag{2.12}$$

the second of which coincides with (2.11) for $\nu = 1$ in this case. Also, for $\nu = 2$, (2.11) is an identity and thus the condition

$$\sum_{j=0}^{k} \alpha_j \tau_j^2 = 2 \sum_{j=0}^{k} \beta_j \tau_j \tag{2.13}$$

added to (2.12) guarantees second-order accuracy for both (2.7) and (2.8).

Consider now the general two-step formula, *i.e.* (2.1) for $k = 2$ with $t_n^* = t_{n+1}$, $\tau_1 = \tau_{1,n} = 0$, and with $\tau_0 = \tau_{0,n}$, $\tau_2 = \tau_{2,n}$ defined by

$$\begin{aligned} h_{n+1} &= t_{n+1} - t_n = -\tau_0 \bar{h}_n, \\ h_{n+2} &= t_{n+2} - t_{n+1} = \tau_2 \bar{h}_n. \end{aligned} \tag{2.14}$$

In this case the consistency conditions (2.12) become

$$\rho(1) = \alpha_0 + \alpha_1 + \alpha_2 = 0,$$
$$\alpha_0\tau_0 + \alpha_2\tau_2 = 1 \tag{2.15}$$

In addition, the constraint

$$\rho'(1) := \sum_{j=0}^{2} j\alpha_j = \sigma(1) \tag{2.16}$$

is being imposed for the purpose of pinning down $\hat{h}_n$, τ_0 and τ_2 (see (2.24) hereafter). Relation (2.16) is reminiscent of the first-order consistency condition (2.12b) but is equivalent to that condition only in the case of equal steps, *i.e.* when $h_{n+1} = h_{n+2} = \hat{h}_n = h$ and $-\tau_0 = \tau_2 = 1$.

From (2.15) and (2.16) it follows that $\sigma(\zeta)/\rho(\zeta) = s(z)/r(z) \sim \frac{1}{2}z$ for $z := (\zeta + 1)/(\zeta - 1) \to \infty$ (*i.e.* as $\zeta \to 1$); here $r(z) := (z-1)^2\rho(\zeta(z))$, $s(z) := (z-1)^2\sigma(\zeta(z))$, and $\zeta(z) = (z+1)/(z-1)$. Hence there exist quantities a, b, and c such that

$$2\sigma(\zeta(z))/\rho(\zeta(z)) = z + \frac{az+b}{z+c} \tag{2.17}$$

and

$$\alpha_2 = \frac{1}{2}(c+1) \quad , \quad \beta_2 = \frac{1}{4}[1 + b + (a+c)],$$
$$\alpha_1 = -c \quad , \qquad \beta_1 = \frac{1}{2}(1-b), \tag{2.18}$$
$$\alpha_0 = \frac{1}{2}(c-1) \quad , \quad \beta_0 = \frac{1}{4}[1 + b - (a+c)]$$

By (2.12), (2.13) and (2.18) the first- and second-order accuracy constraints can be rewritten as

$$(c+1)\tau_2 + (c-1)\tau_0 = 2, \tag{2.19}$$

$$(c+1)\tau_2^2 + (c-1)\tau_0^2 = (1+b)(\tau_2 + \tau_0) + (a+c)(\tau_2 - \tau_0) \tag{2.20}$$

The variability of the step size can be represented by the parameter

$$\alpha := c(\tau_0 + \tau_2)/2 \tag{2.21}$$

which vanishes for equal steps. From (2.19) and (2.21) we get

$$\tau_2 - \tau_0 = 2(1-\alpha). \tag{2.22}$$

The second-order accuracy condition (2.20), which is equivalent to

$$c[(\tau_2 + \tau_0)^2 + (\tau_2 - \tau_0)^2] + 2(\tau_2 + \tau_0)(\tau_2 - \tau_0) = 2(1 + b)(\tau_2 + \tau_0) + 2(a + c)(\tau_2 - \tau_0),$$

can thus be rewritten as

$$c[(4\alpha^2/c^2) + 4(1-\alpha)^2] + 8(1-\alpha)\alpha/c = 4(1 + b)\alpha/c + 4(a + c)(1-\alpha),$$

or

$$(\alpha - \alpha^2)(1-c^2) = b\alpha + ac(1-\alpha).$$

For $\alpha = 0$ (equal steps) and $c \neq 0$, this last condition reduces to $a = 0$, and for $\alpha(1-\alpha) \neq 0$ it can be written in the form

$$\frac{ac}{\alpha} + \frac{b}{1-\alpha} = 1 - c^2. \tag{2.23}$$

From (2.14), (2.21) and (2.22) it follows that

$$\begin{aligned} \tau_2 &= 1 - \alpha + \frac{\alpha}{c}, \\ -\tau_0 &= 1 - \alpha - \frac{\alpha}{c}, \\ \bar{h}_n &= h_{n+2}/\tau_2 = h_{n+1}/(-\tau_0). \end{aligned} \tag{2.24}$$

The formal *algebraic condition for A-stability*,

$$Re\, \rho(\zeta)/\sigma(\zeta) \geq 0 \quad \text{for} \quad |\zeta| \geq 1,$$

is equivalent to

$$Re\, r(z)/s(z) \geq 0 \quad \text{for} \quad Re\, z \geq 0,$$

i.e. that $r(z)/s(z)$ be a positive function [9]; here $r(z) = 2(z + c)$ and $s(z) =$

$z(z+c)+az+b$. From (2.17) it follows that this condition is satisfied iff

$$a \geq 0, \quad b \geq 0, \quad c \geq 0. \tag{2.25}$$

An interpretation of the condition (2.25) as an actual (not just formal) stability result is given in Section 5 hereafter. It is useful in the following to carry out the investigation of A-contractivity subject to this constraint.

To analyze A-contractivity of (2.1) in the G-norm, recall [7] that the determination of a G-matrix is related to decompositions of the form

$$Re\ \frac{1}{2}r(z)\overline{s(z)} = (|m_1 z + m_0|^2 + n_0)x + |\psi_1(z)|^2 + |\psi_0(z)|^2, \tag{2.26}$$

where $x = Re\ z$, $m_1 > 0$, $n_0 > 0$, and ψ_0, ψ_1 are linear functions. In fact,

$$G = P^T \hat{G} P, \tag{2.27}$$

where

$$\hat{G} = \begin{bmatrix} m_0^2 + n_0 & m_1 m_0 \\ m_1 m_0 & m_1^2 \end{bmatrix}, \quad P = \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}.$$

Note that $\hat{G}$ is positive definite. In homogenous coordinates P corresponds to the Moebius transform $z = (\zeta+1)/(\zeta-1)$. Put for brevity,

$$\hat{G} := \begin{bmatrix} g_{11} & g_{12} \\ g_{12} & g_{22} \end{bmatrix}.$$

We may write (2.26) in the form

$$Re\ \frac{1}{2}r(z)\overline{s(z)} = (1, \bar{z}, \bar{z}^2)(\frac{1}{2}\overline{G} + H)(1, z, z^2)^T \tag{2.28}$$

where H is a positive semi-definite matrix, the elements of which are determined by the polynomials ψ_1, ψ_0.

$$\overline{G} = \begin{bmatrix} 0 & g_{11} & g_{12} \\ g_{11} & 2g_{12} & g_{22} \\ g_{12} & g_{22} & 0 \end{bmatrix}, \quad H = \begin{bmatrix} h_{11} & h_{12} & 0 \\ h_{12} & h_{22} & 0 \\ 0 & 0 & 0 \end{bmatrix} \geq 0.$$

One decomposition of the form (2.26) is easily found, namely

$$Re[\frac{1}{2}r(z)\overline{s(z)}] \equiv Re\{(z+c)[\bar{z}(\bar{z}+c)+a\bar{z}+b]\} = |\,|z+c|^2+(ac+b)|c+a|z|^2+bc.$$

In this *special case* we obtain,

$$\hat{G}_{spec} = \begin{bmatrix} c^2+ac+b & c \\ c & 1 \end{bmatrix}, \quad H_{spec} = \begin{bmatrix} bc & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

We are interested in all possible decompositions of the form (2.26) or, equivalently, (2.28). It follows from (2.28) and the form of $\bar{G}$ and H that h_{11}, $g_{11}+2h_{12}$, g_{12} *etc.* are the same for all such decompositions. Hence,

$$h_{11} = bc,\ g_{12} = c,\ g_{22} = 1,\ h_{22} = a,\ 2h_{12} = c^2+ac+b-g_{11}$$

In addition to this, we have the positivity conditions for $\hat{G}$ and H. Put for brevity $g_{11} = g$. Then

$$\hat{G} = \begin{bmatrix} g & c \\ c & 1 \end{bmatrix}, \quad g > c^2 \tag{2.29}$$

and

$$abc \geq h_{12}^2 = \frac{1}{4}(c^2+ac+b-g)^2. \tag{2.30}$$

The matrix G associated with $\hat{G}$ of (2.29) is

$$G = \begin{pmatrix} 1+g-2c & 1-g \\ 1-g & 1+g+2c \end{pmatrix}; \tag{2.31}$$

it is subject to the constraints $g > c^2$ and (2.30).

Global A-contractivity (and thus A-stability) results are obtained, for all solutions of monotone nonlinear systems [6] generated by variable-step one-leg methods of type (2.8), if for all $n \geq 0$ the formula (2.1) is A-contractive in a G-norm with a G which is *independent* of n (*i.e.* of the step ratio). For G of (2.31) to be independent of n, g and c must be constant. The latter means that the difference operator ρ defined by (2.4) is constant with respect to n.

From this point on the analysis will be restricted to second-order formulas, *i.e.* formulas for which (2.23) holds. Since in this case $a \to 0$ if $\alpha \to 0$, (2.30) implies that

$g - c^2 - b(0) = 0$ and that

$$b(\alpha) + a(\alpha)c - g + c^2 = O(|a(\alpha)|^{1/2}), \quad \alpha \to 0.$$

Hence $b(\alpha)$ is continuous at $\alpha = 0$. From (2.23) it follows that

$$b(0) = 1 - c^2 - c \lim_{\alpha \to 0} (a/\alpha)$$

i.e. $\lim_{\alpha \to 0} (a/\alpha)$ exists. Since $a \geq 0$ for $|\alpha| << 1$ because of the A-stability requirements, it follows that $\lim_{\alpha \to 0} (a/\alpha) = 0$ (since the right limit is ≥ 0 and the left limit is ≤ 0). Hence $b(0) = 1 - c^2$, $g = 1$, and the only possible choice for G is

$$G = 2\begin{pmatrix} 1-c & 0 \\ 0 & 1+c \end{pmatrix}, \quad 0 < c < 1, \tag{2.32}$$

a *diagonal* matrix.

If in (2.30) one lets $g = 1$ and uses the second-order accuracy condition (2.23) to express ac in terms of b, α, and c^2 then, in this case, (2.30) becomes

$$-|(1-\alpha)(1-c^2) - \frac{b}{1-\alpha}|^2 \geq 0 \tag{2.33}$$

Therefore, the only second-order methods which are A-contractive in a fixed G-norm for arbitrary step ratios are defined by

$$\begin{aligned} a(\alpha) &= (1-c^2)\alpha^2/c, \\ b(\alpha) &= (1-c^2)(1-\alpha)^2, \\ c(\alpha) &= c = const, \quad 0 < c < 1. \end{aligned} \tag{2.34}$$

Another way of arriving at the one-parameter class of methods (2.34) is to observe [10] that for any fixed c the equation (2.23) defines a one-parameter family of straight lines in the plane with cartesian coordinates (ac, b). The envelope of this family is given by (2.34). As mentioned above, in order to have a G-norm independent of n, the difference operator ρ must be fixed.

3. A-contractivity in the ℓ_∞-norm

In the preceding section it was shown that the class of all second-order two-step formulas with variable steps which are A-contractive in the G-norm is defined by (2.34). Here it will be proved that this same class also represents all variable-step $p = k = 2$ formulas which are A-contractive in the ℓ_∞-norm. However, as will be seen, the requirement that the operator ρ be constant with respect to n which had to be imposed in analyzing A-contractivity in the G-norm may be dropped in studying the same property in the ℓ_∞-norm.

Let $h^- := h_{n+1} = t_{n+1} - t_n$, $h^+ := h_{n+2} = t_{n+2} - t_{n+1}$, and $h := \frac{1}{2}(h^+ + h^-)$. Then one has $h^+ = h(1+\epsilon)$ and $h^- = h(1-\epsilon)$, where $\epsilon = (h^+ - h^-)/2h$, $-1 < \epsilon < +1$; *i.e.* $\epsilon = 0$ for equal steps ($h^- = h^+$). For bounded step ratios, one has the following expressions for the first and second central divided differences of any sufficiently smooth function $x(t)$:

$$\left(\frac{\delta x(t)}{\delta t}\right)_{t=t_{n+1}} := \frac{1}{2(1-\epsilon^2)h}[-(1+\epsilon)^2 x(t_n) + 4\epsilon x(t_{n+1}) + (1-\epsilon)^2 x(t_{n+2})] = \dot{x}(t_{n+1}) + O(h^2),$$

$$\left(\frac{\delta^2 x(t)}{\delta t^2}\right)_{t=t_{n+1}} := \frac{1}{(1-\epsilon^2)h^2}[(1+\epsilon)x(t_n) - 2x(t_{n+1}) + (1-\epsilon)x(t_{n+2})] = \ddot{x}(t_{n+1}) + O(h). \tag{3.1}$$

If unsubscripted quantities are assigned to t_{n+1}, then one can write a normalized ansatz for a two-step formula in divided difference form:

$$u_0 x + u_1 h\frac{\delta x}{\delta t} + u_2 h^2 \frac{\delta^2 x}{\delta t^2} - h\left(\dot{x} + v_1 h\frac{\delta \dot{x}}{\delta t} + v_2 h^2 \frac{\delta^2 \dot{x}}{\delta t^2}\right) = 0 \tag{3.2}$$

In order for (3.2) to be consistent (of order of accuracy $p = 1$) it must be satisfied exactly for $x(t) \equiv 1$ and $x(t) = t$. This is the case iff $u_0 = 0$ and $u_1 = 1$. The class of all consistent formulas can thus be written in terms of the three parameters $u = u_2$, $v = v_1$, and $w = v_2$ as follows:

$$h\frac{\delta x}{\delta t} + uh^2\frac{\delta^2 x}{\delta t^2} - h\left(\dot{x} + vh\frac{\delta \dot{x}}{\delta t} + wh^2\frac{\delta^2 \dot{x}}{\delta t^2}\right) = 0. \tag{3.3}$$

The $p = 2$ accuracy condition, gotten from substituting $x(t) = t^2$ into (3.3), is simply

$$u = v. \tag{3.4}$$

If from (3.1) one substitutes for the divided differences and groups terms one finds the following expressions for the formula coefficients

$$
\begin{aligned}
\alpha_0 &= \gamma-\delta, & \beta_0 &= \phi-\psi, \\
\alpha_1 &= -2\gamma, & \beta_1 &= 1-2\phi, \\
\alpha_2 &= \gamma+\delta, & \beta_2 &= \phi+\psi,
\end{aligned}
\tag{3.5}
$$

where

$$
\begin{aligned}
\gamma &:= \frac{-2\epsilon+2u}{2(1-\epsilon^2)}, & \delta &:= \frac{1+\epsilon^2-2\epsilon u}{2(1-\epsilon^2)}, \\
\phi &:= \frac{-2\epsilon v+2w}{2(1-\epsilon^2)}, & \psi &:= \frac{(1+\epsilon^2)v-2\epsilon w}{2(1-\epsilon^2)}.
\end{aligned}
\tag{3.6}
$$

Two identities are implied by these definitions:

$$
\begin{aligned}
1-2\epsilon\gamma &= 2\delta, \\
\epsilon\phi+\psi &= \frac{1}{2}v.
\end{aligned}
\tag{3.7}
$$

Note that the normalization is again (2.2), *i.e.* $\sum_{j=0}^{2}\beta_j = 1$.

The class of formulas defined by (3.5) and (3.6) is the same as that defined in terms of the parameters a, b, c by (2.18). The transformation $(u, v, w) \rightarrow (a, b, c)$ and that of related quantities can be found by requiring that $\sigma_{a,b,c} \equiv \sigma_{u,v,w}$ and $\rho_{a,b,c}/\bar{h} \equiv \rho_{u,v,w}/h$, where $\bar{h} = \tilde{h}_n$. One obtains the relations

$$
\begin{aligned}
a &= 4\psi-c = 4\psi-(\gamma/\delta), \\
b &= 4\phi-1, \\
c &= \gamma/\delta, \\
\alpha &= 2\epsilon\gamma = 1-2\delta, \\
\bar{h} &= h/2\delta, \\
\tau_2 &= 2(1+\epsilon)\delta, \\
-\tau_0 &= 2(1-\epsilon)\delta.
\end{aligned}
\tag{3.8}
$$

In the present parametrization, $r(z) = 4(\delta z+\gamma)$ and $s(z) = z^2+4\psi z+(4\phi-1)$. By applying the result of Example 2, p.13 of [9] to $s(z)/r(z)$ one finds the formal A-stability conditions

$$\delta > 0,$$

$$\phi \geq \frac{1}{4}, \tag{3.9}$$

$$0 \leq \gamma \leq 4\delta\psi.$$

It was proved in [18] that a multistep formula is A_0-contractive in the max norm (ℓ_∞-norm) iff

$$\alpha_k > 0, \ \alpha_j \leq 0, \ j = 0, \ldots, k-1,$$
$$\beta_k - \sum_{j=0}^{k-1} |\beta_j| \geq 0. \tag{3.10}$$

A formula is A-contractive in the max norm iff both (3.10) and

$$\sum_{j=0}^{k-1} R_j(\eta) \leq 1, \ 0 \leq \eta < +\infty, \tag{3.11}$$

are satisfied, where

$$R_j(\eta) = \left[(\alpha_j^2 + \beta_j^2\eta)/(\alpha_k^2 + \beta_k^2\eta)\right]^{1/2}, \ j = 0, \ldots, k-1, \tag{3.12}$$

and where the square roots are positive by definition. For $k = 2$ it is feasible to reduce (3.11) to a condition just involving the formula coefficients. In fact, $R_0 + R_1 \leq 1 \iff 2R_0R_1 \leq 1 - R_0^2 - R_1^2 \iff 4R_0^2R_1^2 \leq (1 - R_0^2 - R_1^2)^2$, the last inequality being rational. This latter is in turn equivalent to a condition of the form $p_0 + p_1\eta + p_2\eta^2 \geq 0$, $\eta \geq 0$, in which $p_0 = 0$ by consistency and $p_2 \geq 0$ by (3.10). Therefore, a two-step formula is A-contractive in the max norm iff both (3.10) and

$$p_1 := (\alpha_2^2 - \alpha_1^2 + \alpha_0^2)(\beta_2^2 - \beta_1^2 + \beta_0^2) - 2(\alpha_2^2\beta_0^2 + \alpha_0^2\beta_2^2) \geq 0 \tag{3.13}$$

hold. After substitution from (3.5), a calculation gives the condition

$$\frac{1}{2}p_1 = (\delta^2 - \gamma^2)(4\phi - 1) - 4(\gamma\psi - \delta\phi)^2 \geq 0 \tag{3.14}$$

which is equivalent to (3.13). Using the notations $A := -r/(1-r^2)$, $B := (1-r^2)^{-1}$, and $C := (1 + r^2)/2(1-r^2)$ and the second-order accuracy condition (3.4), one has $\gamma = A + B\nu$,

$\delta = C + Av$, $\phi = Av + Bw$, and $\psi = Cv + Aw$. Another calculation yields $\delta^2 - \gamma^2 = \frac{1}{4} - Av - Bv^2$, $4\phi - 1 = 4Av + 4Bw - 1$, $4(\gamma\psi - \delta\phi)^2 = [B(w - v^2)]^2$, and thus (3.14) finally takes the form

$$\frac{1}{2}p_1 = -\frac{1}{4}\left[(1 - 4Av) - 2B(w + v^2)\right]^2 \geq 0.$$

This last condition is satisfied iff $w = (2B)^{-1} - (2A/B)v - v^2$, i.e. iff

$$w = \frac{1 - \epsilon^2}{2} + 2\epsilon v - v^2 = \frac{1 + \epsilon^2}{2} - (\epsilon - v)^2 \qquad (3.15a)$$

As will be shown in the next section, (3.10) implies that of the parabola (3.15a) only the arc defined by

$$\epsilon < v \leq \frac{1 + \epsilon}{2}, \quad -1 < \epsilon < 1, \qquad (3.15b)$$

corresponds to A-contractive methods. It can be verified, by using the transformation (3.8), that the class of second-order formulas defined by (2.34) is the same as that defined by (3.3), (3.4) and (3.15).

Remark: The use of the ℓ_v-norm is natural since it is the only norm in which all of the formulas defined by the interval (3.15b), including its endpoints the Trapezoidal Rule ($v = (1 + \epsilon)/2$) and the two-step Trapezoidal Rule ($v = \epsilon$), are simultaneously A-contractive ([20], Proposition 2.4).

4. A_0-contractivity and summary of methods

It was proved in [18] that, in the ℓ_∞-norm, the formula (2.1) is a) contractive at $q = 0$ iff

$$\alpha_j \leq 0, \; j = 0, \ldots, k-1, \; \alpha_k > 0, \tag{4.1}$$

b) contractive at $q = \infty$ iff

$$\hat{\gamma} = \beta_k - \sum_{j=0}^{k-1} |\beta_j| \geq 0, \tag{4.2}$$

and c) A_0-contractive iff both (4.1) and (4.2) hold (as stated earlier). For the class of formulas with $p = k = 2$ defined by (3.4)-(3.6), $\alpha_0 \leq 0$ and $\alpha_1 \leq 0$ yield

$$\epsilon \leq \nu \leq \frac{1+\epsilon}{2}. \tag{4.3}$$

The condition $\alpha_2 > 0$, which is equivalent to $\nu > -(1-\epsilon)/2$, is implied by (4.3). In discussing (4.2) one distinguishes four cases depending on the signs of β_0 and β_1. First note that $\beta_0 \gtrless 0$ iff

$$w \gtrless \frac{1+\epsilon}{2} \nu \tag{4.4}$$

and $\beta_1 \gtrless 0$ iff

$$w \lessgtr \frac{1-\epsilon^2}{2} + \epsilon\nu. \tag{4.5}$$

Case 1: For $\beta_0 \geq 0$ and $\beta_1 \geq 0$ one has $\hat{\gamma} = \beta_2 - \beta_0 - \beta_1 = 2(\phi + \psi) - 1 \geq 0$ iff

$$w \geq \frac{1+\epsilon}{2} - \frac{1-\epsilon}{2} \nu. \tag{4.6}$$

Case 2: For $\beta_0 < 0$ and $\beta_1 \geq 0$, $\hat{\gamma} = \beta_2 + \beta_0 - \beta_1 = 4\phi - 1 \geq 0$ iff

$$w \geq \frac{1-\epsilon^2}{4} + \epsilon\nu. \tag{4.7}$$

But (4.7) and (4.4) require that

$$\frac{1-\epsilon^2}{4} + \epsilon\nu < \frac{1+\epsilon}{2} \nu$$

which implies $v > (1 + \epsilon)/2$. This latter condition is incompatible with (4.3), so that Case 2 does contribute any feasible points to the region of A_0-contractivity in the parameter plane.

Case 3: For $\beta_1 < 0$ and $\beta_0 \geq 0$, $\hat{\gamma} = \beta_2 - \beta_0 + \beta_1 = 2(\psi - \phi) + 1 \geq 0$, *i.e.*

$$w \leq \frac{1+\epsilon}{2} v + \frac{1-\epsilon}{2} \tag{4.8}$$

Case 4. For $\beta_1 < 0$ and $\beta_0 < 0$, an argument similar to that of Case 2 shows that there are no A_0-contractive methods of this type. The region of A_0-contractivity in the plane of the parameters (w, v) is the shaded triangle shown in Figure 1 for increasing steps ($\epsilon = \frac{1}{5}$) and in Figure 2 for decreasing steps ($\epsilon = -\frac{1}{5}$). The line $\beta_1 = 0$ divides this triangle into two subtriangles; the left hand one represents the contribution from Case 1, the right hand one that from Case 3. The upper left and lower vertices of the A_0-contractivity triangles represent (identically in ϵ), the Trapezoidal Rule (TR), defined by $\alpha_0 = \beta_0 = 0$ and the two-step Trapezoidal Rule (2TR), having $\alpha_1 = \beta_1 = 0$. The set of all second-order A-contractive methods (both in the G-norm and in the ℓ_∞-norm), defined by (2.34) respectively by the equivalent relations (3.15), is represented by arcs of parabolas in Figures 1 and 2, joining TR and 2TR.

One may ask whether it is possible to select a particular formula from among the A_0-contractive or the A-contractive ones whose truncation error is in some sense minimal? Of course, there is no unique way of making such a choice. If the problem is smooth and no dissipation is required, the TR (resp. its one-leg counterpart, the Implicit Midpoint Rule) or a method "close" to it may be the right choice, while for rough problems one needs a considerable amount of dissipation which one can provide by asking for strong contractivity at $q = \infty$. In [19] a compromise choice of an A_0-contractive formula was made by minimizing, over all A_0-contractive formulas with $p = k = 2$, a bound for the global truncation error produced if an $A(0)$-contractive formula is implemented as a one-leg method and applied to the test problem $\dot{x} = \lambda(t)x$, $\lambda(t) \leq -a$, $a > 0$. The calculation was restricted to fixed integration steps. It resulted in finding an A_0-contractive (indeed, $A(\alpha)$-contractive) formula of Adams type,

$$x_{n+2} - x_{n+1} - h\left(\frac{3}{4}\dot{x}_{n+2} + \frac{1}{4}\dot{x}_n\right) = 0, \tag{4.9}$$

which in [19] was referred to as *CA2*. A unique generalization of (4.9) to arbitrary variable steps was then defined by requiring that the variable-step version represent a second-order accurate Hermite interpolation formula of the same form as (4.9), *i.e.* with $\alpha_0 = \beta_1 = 0$, and it was proved that the variable-step version defined in this manner, when implemented as a one-leg method, remained A_0-contractive (in the max norm) for any $\lambda(t) \leq 0$ and for any step sequence $\{h_n\}$ whatsoever. For a given k the objective function, whose minimization over the two-parameter set of all A_0-contractive formulas led to (4.9), was $|c_3|/\hat{\gamma}$; here c_3 is the error constant and $\hat{\gamma} = \beta_k - \sum_{j=0}^{k-1} |\beta_j|$ is the contractivity constant considered in (3.10) and (4.2), both of which are functions of the parameters. It can be shown - although it was not stated in [19] - that formally minimizing $|c_3|/\hat{\gamma}$ over all A_0-contractive formulas in the variable step case defines the same generalization of (4.9) as does the Hermite interpolation requirement mentioned before. The variable step version of (4.9) is defined by (4.19) hereafter in the form given in [19] which is practical for numerical computation. It is represented in Figures 1 and 2 by the point labeled OPA_0 (for "optimal" A_0-contractive method), the intersection of the lines $\alpha_0 = \beta_1 = 0$.

The transformation

$$w(\epsilon) = \frac{(1+\epsilon)[(1+\epsilon^2)w(0) - \epsilon^2 v(0)]}{(1-\epsilon)+2\epsilon[2w(0)-v(0)]},$$

$$v(\epsilon) = \frac{(1-\epsilon)[2\epsilon w(0)+(1-2\epsilon)v(0)]}{(1-\epsilon)+2\epsilon[2w(0)-v(0)]}, \tag{4.10}$$

maps the triangle representing the A_0-contractive formulas for $\epsilon = 0$ one-to-one onto the corresponding triangle for any $\epsilon \neq 0$. The lines $\alpha_0 = \beta_0 = \beta_1 = 0$ are invariants of this transformation and thus the fixed- and variable-step versions of OPA_0 and of the backward differentiation formula (BDF) correspond to one another.

We derived a particular A-contractive $p = k = 2$ formula for arbitrary step ratio which minimizes the objective function $|c_3|/\hat{\gamma}$ mentioned in the preceding paragraph. The error constant for the $p = k = 2$ formula associated with (v, w) turns out to be

$$c_3 = \frac{1}{6}\left[(1-\epsilon^2) + 4\epsilon v - 6w\right]; \tag{4.11}$$

on the class (3.15) one finds that $|c_3| = \frac{1}{3}\left[(1+\epsilon^2) + 4\epsilon v - 3v^2\right]$. A calculation shows that $|c_3(v)|/\hat{\gamma}(v)$ takes its global minimum at

$$v_{opt} = (1+\epsilon)^2(3+\epsilon)^{-1} \tag{4.12a}$$

which is an interior point of the interval defined by (3.15b) for all $\epsilon, -1 < \epsilon < 1$. The value of w, corresponding to v_{opt} via (3.15a), is

$$w_{opt} = \frac{1}{2}(1 + \epsilon)(7 + 3\epsilon + 5\epsilon^2 + \epsilon^3)/(3 + \epsilon)^2. \tag{4.12b}$$

For equal steps ($\epsilon = 0$), the particular A-contractive formula defined by (4.12) is

$$-\frac{1}{6}x_n - \frac{4}{6}x_{n+1} + \frac{5}{6}x_{n+2} - h\Big(\frac{2}{9}\dot{x}_n + \frac{2}{9}\dot{x}_{n+1} + \frac{5}{9}\dot{x}_{n+2}\Big) = 0. \tag{4.13}$$

It is represented in Figures 1 and 2 by the points labeled OPA for ("optimal" A-contractive method).

For practical use the family of variable-step $p = k = 2$ methods studied in Sections 2 and 3 is rewritten hereafter, with $n-2$ replacing n, in terms of the forward step $h_n = t_n - t_{n-1}$ (rather than the average step $h = \frac{1}{2}(h_n + h_{n-1})$ used in Section 3) and in terms of the step ratio $r = r_n = h_n/h_{n-1}$ (rather than $\epsilon = (h_n - h_{n-1})/2h$). The relationship between r and ϵ is

$$r = \frac{1+\epsilon}{1-\epsilon} \quad \longleftrightarrow \quad \epsilon = \frac{r-1}{r+1} \tag{4.14}$$

The class of formulas defined by (3.5) and (3.6) (or (2.18)) is equivalent to

$$\alpha_0 x_{n-2} + \alpha_1 x_{n-1} + \alpha_2 x_n - h_n(\beta_0 \dot{x}_{n-2} + \beta_1 \dot{x}_{n-1} + \beta_2 \dot{x}_n) = 0, \tag{4.15}$$

where the coefficients

$$\begin{aligned}
\alpha_0 &= -\frac{r^2}{1+r}(1-b_1) \quad , \quad \beta_0 = \frac{r^2}{2(1+r)}(1 + b_0 - b_1), \\
\alpha_1 &= -[1 - r(1-b_1)] \quad , \quad \beta_1 = (1 - \frac{1}{2}b_1) - \frac{r}{2}(1 + b_0 - b_1), \\
\alpha_2 &= 1 - \frac{r}{1+r}(1-b_1) \quad , \quad \beta_2 = \frac{1}{2}b_1 + \frac{r}{2(1+r)}(1 + b_0 - b_1),
\end{aligned} \tag{4.16}$$

depend on n via the step ratio $r = r_n$ and possibly via the parameters b_0, b_1 which may also vary with n. The parameters v and w of Section 3 relate to b_0, b_1 as follows:

$$\begin{aligned}
v &= \frac{1+\epsilon}{2} b_1, \\
w &= (\frac{1+\epsilon}{2})^2 (1 + b_0).
\end{aligned} \tag{4.17}$$

The use of b_0 and b_1 is motivated by the fact that for $r = 1$ (equal steps) one has $s(z) = \sigma(z(\zeta)) = b_0 + b_1 z + z^2$ and the A-stability set in the parameter plane (b_0, b_1) is the first quadrant. The error constant for the general formula (4.16) is

$$c_3 = \frac{1}{12r}[(2-3r)-3rb_0-(2-2r)b_1]. \tag{4.18}$$

The variable-step version of the optimal A_0-contractive formula (4.10) labeled OPA_0 for which $b_0 = 1/r$ and $b_1 = 1$, is

$$x_n - x_{n-1} - h_n\left[\frac{2+r}{2+2r}\dot{x}_n + \frac{r}{2+2r}\dot{x}_{n-2}\right] = 0 \tag{4.19}$$

and its error constant is

$$c_3 = -\frac{3+r}{12r}. \tag{4.20}$$

The constraint (3.15) (respectively (2.34)) for A-contractivity translates into

$$\begin{aligned} b_0 &= \frac{1}{r^2} - \left(b_1 - \frac{r-1}{r}\right)^2, \\ \frac{r-1}{r} &\le b_1 \le 1. \end{aligned} \tag{4.21}$$

The α-coefficients of the A-contractive formulas are those of (4.16) and the β-coefficients are

$$\begin{aligned} \beta_0 &= \frac{r}{1+r} + \frac{r(r-2)}{2(1+r)}b_1 - \frac{r^2}{2(1+r)}b_1^2, \\ \beta_1 &= \frac{1-r}{2}b_1 + \frac{r}{2}b_1^2, \\ \beta_2 &= \frac{1}{1+r} + \frac{2r-1}{2(1+r)}b_1 - \frac{r}{2(1+r)}b_1^2. \end{aligned} \tag{4.22}$$

The error constant for the A-contractive methods is

$$c_3 = \frac{1}{12r}[-4 + 4(1-r)b_1 + 3rb_1^2]. \tag{4.23}$$

A variable-step extension of the formula OPA given by (4.13) is defined naturally by the relation (4.12a), *i.e.* by requiring that the variable-step version have the same minimality property as the uniform-step version. Condition (4.12a) translates into

$$b_1 = 2r/(2r+1), \tag{4.24}$$

the formula coefficients are

$$\begin{aligned}
\alpha_0 &= -\frac{r^2}{(1+r)(1+2r)}, \\
\alpha_1 &= -\frac{1+r}{1+2r}, \\
\alpha_2 &= \frac{1+2r+2r^2}{(1+r)(1+2r)}, \\
\beta_0 = \beta_1 &= \frac{r(1+r)}{(1+2r)^2}, \\
\beta_2 &= \frac{1+2r+2r^2}{(1+2r)^2},
\end{aligned} \tag{4.25}$$

and the error constant is

$$c_3 = -\frac{(1+r)(1+r+r^2)}{3r(1+2r)^2} \tag{4.26}$$

Another extension of (4.13) is given by the requirement that the variable-step version be A-contractive in the same G-norm as (4.13). Using the notations of Section 3, this requires that $v = v(r) = (1+3r+r^2)/(3+2r)$, resp.

$$b_1(r) = \frac{5r^2-1}{r(5r+1)}. \tag{4.27}$$

Recall that, when formulas are implemented in the one-leg form, the local truncation error consists of two third-order terms. The first of these has the coefficient c_3 and comes from the linear constraints (2.10); the second term is due to the nonlinear constraints (2.11).

5. On variable-step stability

As stated in the Introduction, we seek extensions of uniform-step $p = k = 2$ formulas to arbitrary non-uniform steps whose coefficients α_j, β_j depend smoothly on ϵ near $\epsilon = 0$ (uniform steps) and which generate bounded discrete solutions when applied to the variable coefficient test equation (1.12). A necessary condition for a method to have this property is that it be stable for any geometric step sequence

$$h_n = (1 + \hat{\epsilon})^{n-1}, \ \hat{\epsilon} \text{ constant,} \tag{5.1}$$

for which the step ratio is constant:

$$r = 1 + \hat{\epsilon}, \ \epsilon = \hat{\epsilon}/(2 + \hat{\epsilon}), \tag{5.2}$$

and thus the operators ρ and σ are constant. Furthermore let $\lambda(t)$ be such that

$$\lambda(\sigma t_n) = (1 + \hat{\epsilon})^{1-n} q, \ q \text{ constant}, \ Re\, q \leq 0, \tag{5.3}$$

where, for $t_0 = 0$, $t_n = \sum_{\nu=1}^{n} h_\nu = [(1 + \hat{\epsilon})^n - 1]/\hat{\epsilon}$. Then $q = h_n \lambda(\sigma t_n) =$ constant and the one-leg method generates bounded solutions iff $\rho(\zeta, \epsilon)/\sigma(\zeta, \epsilon)$ satisfies

$$|\zeta| > 1 \Rightarrow Re[\rho(\zeta, \epsilon)/\sigma(\zeta, \epsilon)] > 0. \tag{5.4}$$

Thus (5.4) is a necessary condition for the variable-step, variable-coefficient A-stability property studied here. This condition is satisfied iff (3.9) holds. Assume that the coefficients are smooth enough in ϵ so that we can write $\delta(\epsilon) = \frac{1}{2} - \epsilon v(0) + O(\epsilon^2)$. Then $\delta(\epsilon) > 0$ is obviously satisfied. Furthermore, for arbitrary ϵ, $\gamma(\epsilon) \geq 0$ iff $v(\epsilon) \geq \epsilon$, part of the condition (4.1) for contractivity at $q = 0$. Also, for $|\epsilon| << 1$, $\phi(\epsilon) = w(0) - \epsilon v(0) + O(\epsilon^2)$ and $\phi(\epsilon) \geq \frac{1}{4}$ is equivalent to (4.7), one of the constraints for contractivity at $q = \infty$. Finally, the condition $\gamma(\epsilon) \leq 4\delta(\epsilon)\psi(\epsilon)$ becomes $-\epsilon + v(0) \leq v(0) - 2\epsilon v^2(0) - 2\epsilon w(0) + O(\epsilon^2)$ or, to $O(\epsilon)$, $-\epsilon \leq -2\epsilon v^2(0) - 2\epsilon w(0)$ which is true for any ϵ, $|\epsilon| << 1$, iff

$$w(0) = \frac{1}{2} - v^2(0) \tag{5.5}$$

holds. Condition (5.5), together with (4.7) which for $\epsilon = 0$ is $w(0) \geq \frac{1}{4}$, implies $v(0) \leq \frac{1}{2}$, and $\gamma(0) \geq 0$ requires $v(0) \geq 0$. Thus altogether, for $|\epsilon| << 1$ the necessary condition (5.4) for A-stability is satisfied iff both (5.5) and

$$0 \leq v(0) \leq \frac{1}{2} \tag{5.6}$$

hold which for $\epsilon = 0$ are equivalent to (3.15a), and (3.15b), respectively, defining the A-contractive formulas.

For arbitrary $\epsilon \neq 0$, the formal algebraic A-stability conditions (3.9) yield the constraints derived hereafter. The conditions $\delta > 0$, $\varphi \geq 1/4$, and $\gamma \geq 0$ yield

$$v \underset{>}{<} \frac{1+\epsilon^2}{2\epsilon}, \quad \epsilon \underset{<}{>} 0, \tag{5.7}$$

$$w \geq \frac{1-\epsilon^2}{4} + \epsilon v, \tag{5.8}$$

and

$$v \geq \epsilon, \tag{5.9}$$

respectively. For any ϵ, the constraint $\gamma \leq 4\delta\pi$ takes the form $\epsilon\Phi(v, w, \epsilon) \geq 0$, where

$$\Phi(v, w, \epsilon) := 2[2\epsilon v-(1+\epsilon^2)]w-2(1+\epsilon^2)v^2+\epsilon(3+\epsilon^2)v+(1-\epsilon^2). \tag{5.10}$$

It is satisfied iff $\Phi(v, w, \epsilon) \underset{\leq}{\geq} 0$, $\epsilon \underset{<}{>} 0$. The equality $\Phi(v, w, \epsilon) = 0$ can be written in the form

$$w = [2(1+\epsilon^2)v^2-\epsilon(3+\epsilon^2)v-(1-\epsilon^2)]\{2[2\epsilon v-(1+\epsilon^2)]\}^{-1}, \tag{5.11}$$

a hyperbola whose center lies at $w = (2+\epsilon^2+\epsilon^4)/4\epsilon^2$, $v = (1+\epsilon^2)/2\epsilon$ and whose two asymptotes are $v = (1+\epsilon^2)/2\epsilon$ and $w = [(1+\epsilon^2)/2\epsilon]v + [(1-\epsilon^2)/4\epsilon^2]$. This hyperbola passes through the points $\left(w = \left(\frac{2+\epsilon}{2}\right)^2, v = \frac{1+\epsilon}{2}\right)$ and $\left(w = \frac{1+\epsilon^2}{2}, v = \epsilon\right)$ representing the Trapezoidal Rule (TR) and the two-step Trapezoidal Rule ($2TR$), respectively.

The hyperbola subdivides the (w, v)-plane into a connected set containing the minor axis and into a disconnected set consisting of two branch sets and containing that part of the major axis lying beyond the vertices. For $\epsilon > 0$, the "good" region defined by $\Phi \geq 0$ is the disconnected set. Because the first asymptote is the borderline case of condition (5.7), only one of the branch sets is "allowed" by condition (5.7) and all points of that set do satisfy that condition. Consequently, for $\epsilon > 0$ the set of all points satisfying the formal A-stability conditions is the (bounded) intersection of (5.8), (5.9) and $\Phi \geq 0$. It is represented (for $\epsilon = +1/2$) by the shaded region of Fig. 3 which contains the arc of all A-contractive methods. For comparison with the other figures, the A_0-contractivity triangle is also shown. For $\epsilon < 0$, the "good" region $\Phi \leq 0$ is the connected set. The constraint (5.7) is implied by (5.9) and thus the active constraints are again the same. For $\epsilon = -1/2$, their (unbounded) intersection is represented by the shaded portion of Fig. 4 which again contains the A-contractivity arc.

Figures 3 and 4 indicate that, for ϵ near zero, the arc of the A-contractive formulas nearly coincides with the boundaries of the shaded regions for $\epsilon > 0$, resp. $\epsilon < 0$. Hence assuming smoothness for ϵ near zero, only the methods along the arc are admissible, as we concluded above. However, we have not shown that a non-smooth strategy would not work.

Note that the *BDF*, which for $\epsilon = +1/2$ is (9/8, 3/2) and for $\epsilon = -1/2$ is (1/8, 1/2), lies in the "stable set" only for $\epsilon \leq 0$. It was mentioned in [19] that for the test problem defined by (1.12) and (5.1)-(5.3) with $\lambda(t) \leq 0$, A_0-stability of the *BDF* was lost for $r > 1 + \sqrt{2}$ $\left(\epsilon > \sqrt{2}/(2 + \sqrt{2})\right)$. Indications for instability at smaller step ratios ($r \gtrsim 1.2$) were given in [1] for $\dot{x} = \lambda x$, λ constant, complex, in the sense that for such ratios a sufficient condition for contractivity in a polygonal norm was violated. Here it is shown that for some complex $\lambda(t)$ (oscillatory problems) the *BDF* actually becomes destabilized by the problem defined by (1.12), (5.1) - (5.3) with $r = 1 + \hat{\epsilon}$ for any $\hat{\epsilon} > 0$.

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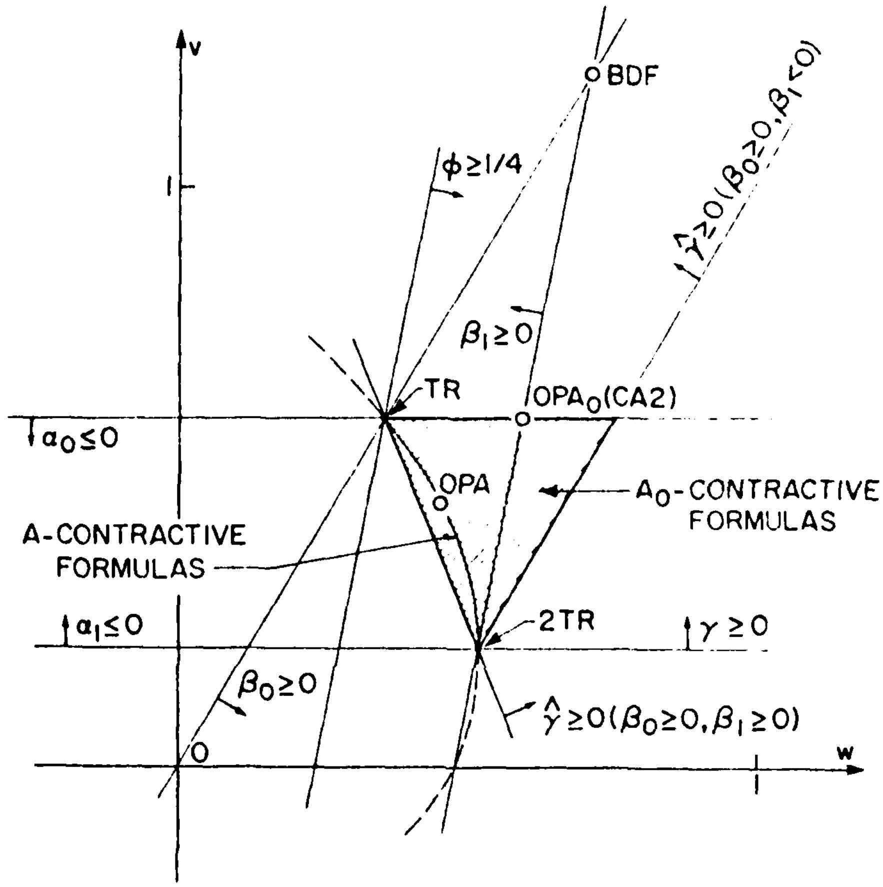

Figure 1. A_0-contractive and A-contractive formulas for increasing steps

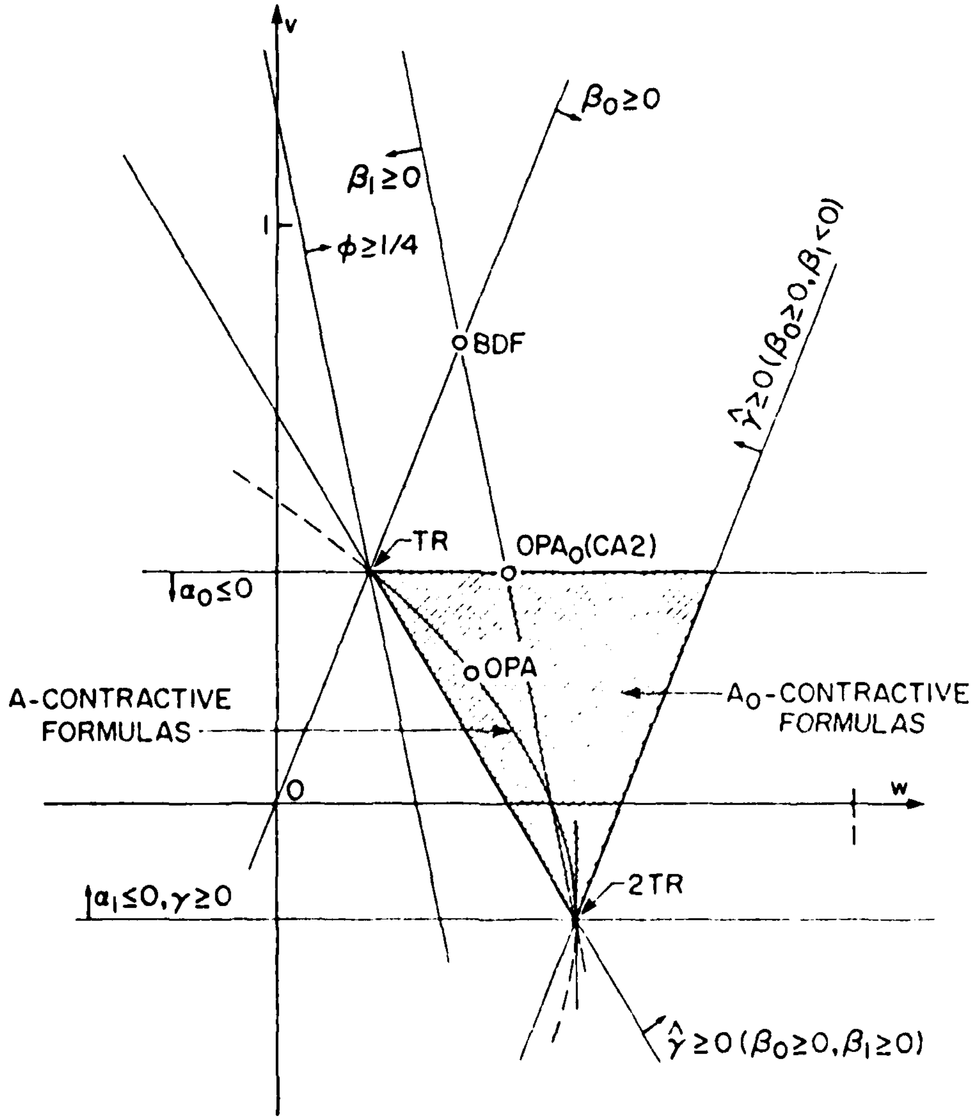

Figure 2. A_0-contractive and A-contractive formulas for decreasing steps.

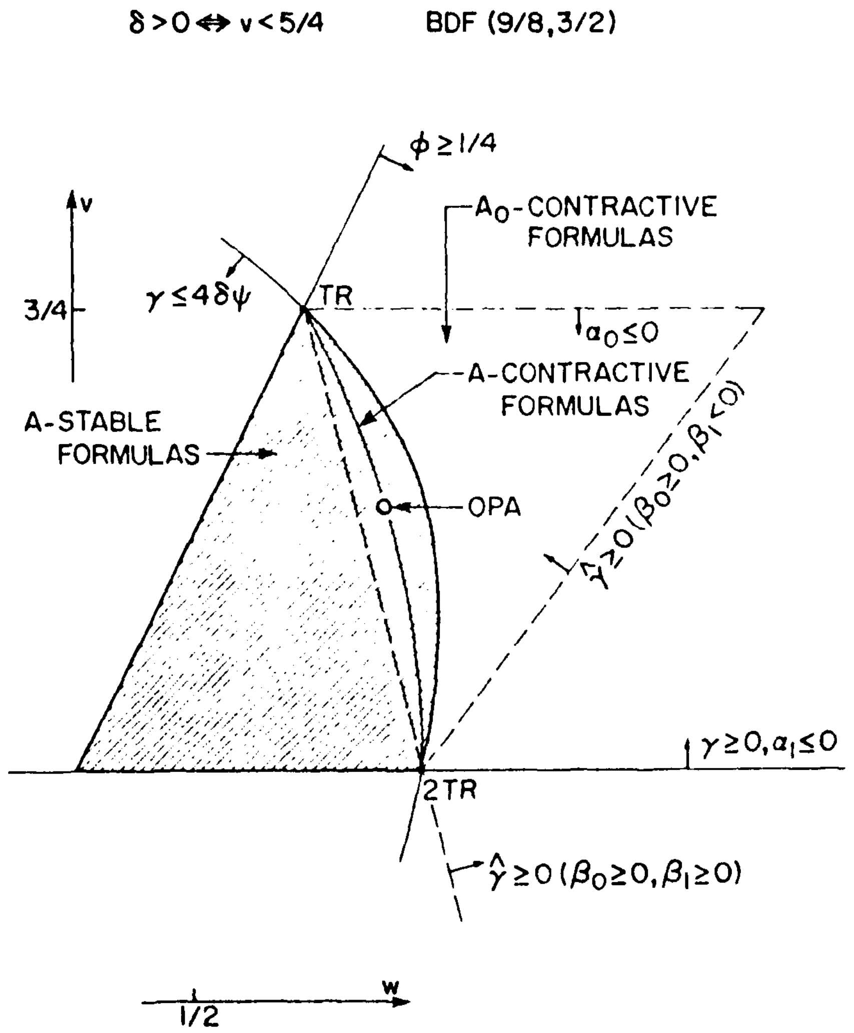

Figure 3. A-stable and A-contractive formulas for increasing steps.

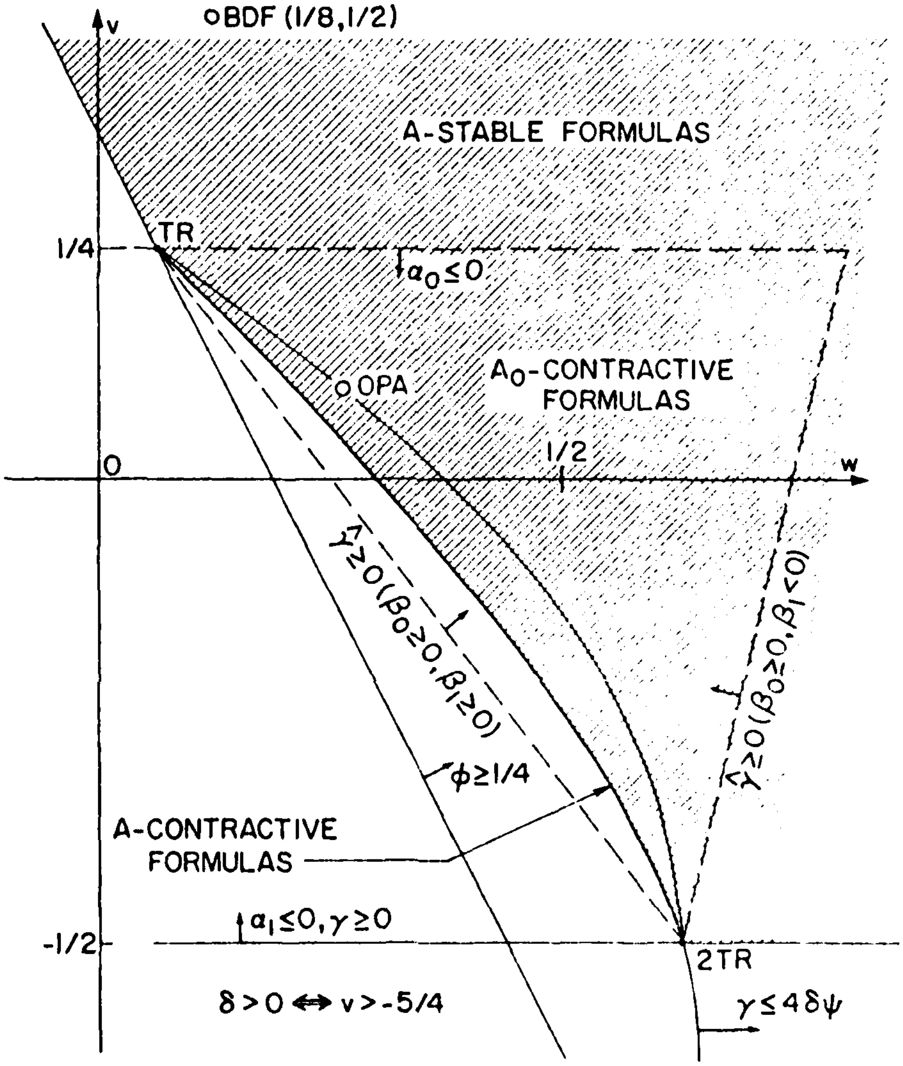

Figure 4. *A*-stable and *A*-contractive formulas for decreasing steps.

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